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Understanding of Nuclear Quadruple Interaction of ^{19}F* and Binding Energies of Solid Fluorine at the First-Principles Level D.R. MISHRA, M.M. ARYAL, TU, Kirtipur,Kathmandu, Nepal, N.P. ADHIKARI, TU, Kirtipur, Kathmandu, Nepal, S.R. BADU, R.H. PINK, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany — We have studied the binding energy (BE) and nuclear quadrupole interaction (NQI) parameters for the ^{19}F* excited nuclear state in solid fluorine as part of our investigation [1] of the properties of solid halogens using the first principles Hartree-Fock Cluster procedure combined with many-body perturbation theory (MBPT), implemented by the Gaussian 03 set of programs. Our results show that Van der Waals interaction obtained from intermolecular electron correlation has dominant effect on the BE but negligible effect on the NQI parameters. For the latter, our e^2qQ is 117.7MHz for$Q(^{19}F^*)$, 0.072 $*10^{-28}m^2$ [2] and η is essentially zero.. The influence of vibrational effects on e^2qQ is being investigated using a first-principles procedure [3] to bridge the small remaining difference with experiment. [1] M.M. Aryal et al., Hyperfine Interact, 176, 51 (2007). [2] K.C.Mishra et al.,Phys. Rev.B25, 3389(1982). [3] N. Sahoo et al. Phys. Rev. Lett. 50, 913(1983) [4] H. Barfuss et al., Phys. Lett. 90A, 33(1982).

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